SOLUTION OF TWO POINT BOUNDARY VALUE PROBLEMS USING QUINTIC HERMITE COLLOCATION METHOD

A

RESEARCH PROPOSAL

SUBMITTED

IN PARTIAL FULFILMENT OF THE REQUIREMENT

FOR

DOCTOR OF PHILOSOPHY

IN

FACULTY OF SCIENCES
DISCIPLINE MATHEMATICS

By

Satinder Pal Kaur
(Enrol. No. 17405FPE02)

MAHARAJA RANJIT SINGH PUNJAB TECHNICAL UNIVERSITY
BATHINDA, PUNJAB, INDIA

(November 2018)

Table of contents

S.no.	Particulars	Page no.
1.	Brief introduction	03 – 05
2.	Literature review	05 – 15
3.	Research gap	15
4.	Problem formulation	15
5.	Research objectives	15 - 16
6.	Contribution and need of the proposed research	16
7.	Methodology	16 – 18
8.	Place of work	18
9.	Facilities required and availability status	18
	Bibliography	18 – 22

1. Brief introduction

Two point boundary value problems are used to describe the chemical engineering processes in a best way. Removal of residual soluble material from fiber or centrifuge cakes by washing is a core problem which frequently occurs in practice. This problem is of considerable practical importance. The displacement of solute from the void space of the bed is associated with a physical dispersion of the washing liquid in the direction of flow. This effect is often referred to as longitudinal dispersion. Longitudinal dispersion and mass transfer in the flowing liquor zone is characterized by the differential equation. A great deal of effort has been applied to compute efficiently the solution of these equations. Another way for simplification of a model is replacing of Partial Differential Equation (*PDE*) by a proper Ordinary Differential Equation (*ODE*).

Two point boundary value problems have been solved analytically and numerically by various methods. Extensive study has been carried out by different authors (Kuo (1960); Brenner (1962); Pellett (1964); Sherman (1964); Grähs (1974); Perron & Lebeau (1977); Rasmuson & Neretnieks (1980); Raghavan & Ruthven (1983); Kim (1989); Trinh, *et al* (1989); Al-Jabari, *et al* (1994); Potůček (1997); Sridhar (1999); Liao & Shiau (2000); Szukiewicz (2000); Liu & Bhatia (1999); Kukreja & Ray (2009))to find the solution of these Boundary Value Problems (BVPs). Besides above, some more authors (Villadsen & Stewart (1967); Fan *et al* (1971); Finlayson (1971); Grähs (1974); Raghavan & Ruthven (1983); Soliman & Ibrahim (1999); Shiraishi (2001)) have used orthogonal collocation method (*OCM*) to solve related problems.

Many other authors such as (Carey & Finlayson (1975); Ma & Guiochon (1991); Arora *et al* (2005, 2006 (a) & (b)); have presented the solution to the models using orthogonal collocation on finite *elements*. Al-Jabari, *et al* (1994); Onah (2002) have given the solution by using Galerkin/Petrov Galerkin method. Prenter (1975); Dyksen & Lynch (2000); Ganaie *et al* (2013); Mittal *et al* (2013) have followed Hermite collocation method. Sun (2000); Gupta & Kukreja (2012) have used Spline Collocation method in solving these models.

Many investigations based on diffusion model of longitudinal mixing in beds of finite length with varying initial and boundary conditions are applicable to displacement washing with axial dispersion and particle *diffusion* are proposed by Grähs (1974) and Brenner (1962) and Kumar *et al* (2010) but with different numerical technique. It is important to mention that the problem for single washer with its simplified version has been solved analytically by Brenner (1962) and Kukreja *et al* (1995) using Laplace transform and numerically using orthogonal

collocation by Grähs (1974) and Arora *et al* (2006a, 2006b). All these methods are very complex and time consuming.

In finite-difference method, however, the solution of the system is very unstable and requires strict selection of step size. Nevertheless, the accuracy of numerical solution is not so high. The discretization of even a few *PDEs* by the method of lines can lead to an extremely large system of *ODEs*; the numerical solution of which may have severe cost and storage implications. The Galerkin method is unsuitable for large systems because the integration process becomes very tedious. Shiraishi (2001) examined the accuracy of the numerical solution to the axial dispersion model by the orthogonal collocation method. Raghavan & Ruthven (1983) also shown that the orthogonal collocation method is better for solving fixed-bed models. Two point boundary value *problems* can also be solved by *pdepe* solver, which is simple, elegant and convenient technique and show a comparable performance.

In *OCM* the choice of trial function is comparatively simple over other weighted residual methods. The collocation points are the zeros of the orthogonal polynomials taken from the expansion of the trial function, enforcing the residual to vanish at the collocation points. It is a very simple, elegant and particularly useful technique for chemical engineering problems. It gained popularity due to less computational time and easy adaptability to the computer programs. Its accuracy is comparable with the analytical one. Also Shiraishi (2001) explained that even for large number of collocation points this type of situation does not hold good results by orthogonal collocation method. Arora *et al* (2006a) developed orthogonal collocation on finite element (*OCFE)* method which gives numerical solutions of the super high-order accuracy. The accuracy in case of *OCFE* is higher than *OCM* but the time consumed is more. With *OCFE* one can solve the partial differential equation by transforming it into a set of differential algebraic equation which can be solved easily. The trial function is usually expressed in terms of Lagrangian interpolation polynomial.

Cubic Hermite collocation method is having the advantage of high order of accuracy and some authors have used Hermite polynomial as a trial function because it does not require a subsidiary condition to make the first derivative continuous. The orthogonal polynomials such as Jacobi, Legendre or Chebyshev are used in the trial function and zeros of these polynomials are taken as collocation points. This technique is used by Ganaie *et al* (2013).

As a modification in the technique of *OCFE*, quintic Hermite as basis function is used in the present method. The domain is divided into finite elements and then *OCFE* with quintic as basis function is applied within each element. As quintic Hermite is C^2 continuous so the condition of continuity of trial function and its first derivative at the nodal points or at the

boundaries of the elements is satisfied. It is worth mentioning here that this technique reduces mathematical complexity and gives even better results.

2. Literature review

The aspiration of pulp and paper industry to produce its target production with high efficiency and less environmental load can only be met by initiating a meticulously planned research on mathematical methods. Most of the researcher described the washing model by coupling the transport equation with various adsorption isotherms to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers. Washing experiments were analysed by trial and error fitting of breakthrough curves. By measuring the exit solute concentration as a function of time, it was possible to construct an exit concentration curve or breakthrough curve. A number of mathematical models have been developed to explain the kinetic behaviour of a fixed-bed adsorber and to estimate the breakthrough curves.

Modeling of pulp washing is done mainly using three approaches namely (a) Process modeling (b) Physical modeling (c) Statistical modeling. Models proposed by earlier investigators can be classified into three categories, namely macroscopic, microscopic and semi quantitative models. The macroscopic models can be categorized as black box type, because these models give outside description of the process based on material balances only. The microscopic models are concerned with the basic mechanism and are based on the fundamentals of fluid dynamics. Semi quantitative models are intermediate between these two models. The microscopic model of packed bed gives importance to three physical rates:

1. Axial dispersion of the bulk fluid (flowing liquor);
2. Intrafiber Fick's second law of diffusion;
3. Liquid phase mass transfer, which accounts for the transport of the solute from the fiber surface to the flowing liquid.

However, boundary conditions describing the solute exchange between the fiber surface and the bulk fluid also play an important role in a general model based on the equation of continuity. The diffusion models involve parameters such as longitudinal dispersion coefficient and mass transfer coefficients.

A lot of literature is available on mathematical models. A complete review of the various process models used to describe pulp washing has been presented by Pekkanen and Norden (1985). Physical models proposed by various investigators such as Lapidus & Amundson (1952), Brenner (1962), Pellett (1964), Sherman (1964), Grähs (1974), Neretnieks (1976),

Perron & Lebeau (1977) has been classified on the basis of mass transfer principles of two types:

1. Differential contact models (macroscopic)
2. Dispersion models (microscopic)

Lapidus & Amundson (1952) have studied the effect of longitudinal diffusion in chromatographic columns and obtained differential equation for the wash liquor. Rasmuson & Neretnieks (1980) described the diffusion in the pore network of the adsorbent with the pore diffusion model. Neretnieks (1976) use the surface diffusion model to interpret the mechanism of the migration of adsorbate through the pore space and pore walls. Initial researchers Brenner (1962) and Sherman (1964) proposed the models based on axial dispersion only. Brenner (1962) studied the washing of filter cake by neglecting the accumulation capacity of fibers and assumed that the phenomena of longitudinal mixing and obtained model in terms of the differential equation. Sherman (1964) has described the overall movement of solute in the bed of non-porous granular material with the diffusion like differential equation by replacing molecular diffusion coefficient with longitudinal dispersion coefficient as molecular diffusion coefficient was found very small as compared to longitudinal dispersion coefficient account for the accumulation (or depletion) capacity of material sorbed by the solids.

Pellet (1966) has introduced a mathematical model combining the effects of particle diffusion and axial dispersion. He has studied the longitudinal dispersion of solute, intra-particle diffusion of solute and liquid-phase mass transfer for the particles of cylindrical and spherical geometry by using modified step function input. Perron & Lebeau (1977) neglected the longitudinal dispersion coefficient to study sodium chloride washing and obtained differential equation for the wash liquor.

Liu & Bhatia (1999) and Raghavan & Ruthven (1983) solved their 2*D* models analytically for linear isotherm. An extensive model related to mass transfer in fibrous particle was given by Grähs (1974), it was also restricted for axial dispersion only. Grähs (1974) has divided the packed bed of cellulose fibers into three different zones namely zone of flowing liquor, stagnant liquor and Moreover certain physical features of the fibers such as fiber porosity and fiber radius were ignored. Al-Jabari *et al* (1994) have followed the Langmuir adsorption isotherm for the deposition of filers on the pulp fibers.

Sridhar (1999) has studied the affinity separation of a packed bed using nonlinear adsorption isotherm. These Models include mass transfer coefficients, film resistance coefficients and porosities of bed and particle. Szukiewicz (2000) has presented a model for diffusion reaction

process. The model was developed using radial coordinates to describe reaction in porous spherical particles. Potŭcek (2005) has followed a linear axial dispersion model to study washing behaviour of pulp fibers and granular particles.

Potŭcek (1997, 2001 & 2005) has followed a linear 1*D* axial dispersion model to study the washing behavior of pulp fibers and granular particles.

Arora and Potŭcek (2009) solved such type of models by neglecting the concentration gradient in the radial direction. Further, Lapidus & Amundson (1952) also followed two adsorption isotherms; one implies that equilibrium is established at each point in the bed while the other assumes the rate of adsorption is finite.

Kim (1989) have proposed two linear driving-force formulas. Kukreja *et al* (2009, 1998 & 1995) have followed axial dispersion model for linear and finite rate isotherms with Danckwert's boundary conditions. The model was verified using industrial data of pulp and paper mill. The experimental data of wheat straw (non wood) was collected from a pulp and paper mill.

2.1. Various Models solved by different authors

The adsorption–desorption, diffusion–dispersion phenomena through a bed of non-porous particles has been represented by various authors using different models. The technique is also studied on two dimensional spaces in axial and radial directions both. The diffusion models involve parameters such as longitudinal dispersion coefficient and mass transfer coefficients. Physical models proposed by various investigators can be classified based on mass transfer principles of two types (i) differential contact models (macroscopic) and the (ii) dispersion models (microscopic).

The mechanics involved are the sum of displacement of the fluid containing solute by movement of water plug controlled by fluid mechanics, dispersion due to back mixing, diffusion due to concentration gradient, and adsorption-desorption due to relative affinity of various solutes towards the particle surface For a systematic analysis of a packed bed of porous particles the bed is macroscopically uniform, particles are of uniform cylindrical size, particle diameter is very small as compared to axial distance, the intra-fiber diffusion coefficient is independent of cake thickness , particle radius and the consistency of fibers and also the particle porosity and bed porosity are interrelated to each other. Most of the researcher described the washing model with various isotherms to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers.

2.1.1 Linear Model

Arora *et al* (2005) studied the washing of filter cake based on the phenomena of longitudinal mixing and assumed it to be governed by Model 1

Model 1

$$\frac{\partial c}{\partial t} = \frac{1}{Pe}\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} \qquad (1(a))$$

Model 2

$$\frac{\partial c}{\partial t} = \frac{1}{Pe}\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} - \frac{\mu Bi}{Pe}c\,, \qquad (1(b))$$

where t is time from commencement of displacement, x is distance from the point of introduction of displacing fluid, $c = c(x,t)$ is solute concentration, Bi represents the Biot number which relates the mass transfer resistance inside and at the surface of the body whereas $\mu = \varepsilon/(1-\varepsilon)$ is the ratio of the volume available for flow to the total volume and ε represents the porosity.

At the inlet to the bed, it is assumed that there is no loss of solute from the bed through the plane at which the displacing fluid is introduced:

$$c = 0 \qquad \text{at } x = 0\,, \qquad (2)$$

At the bed exit, in order to avoid the unacceptable conclusion that the solute concentration passes through a maximum (or minimum) in the interior of the medium, it is necessary to impose the boundary condition:

$$\frac{\partial c}{\partial x} = 0 \qquad \text{at } x = L\,. \qquad (3)$$

Initially, it is assumed that the bulk fluid concentration is equal to the inlet solute concentration, i.e.

$$c(x,0) = 1 \qquad \text{for all } x \qquad (4)$$

Arora *et al* (2006a) has compared the relative error of *OCM* and *OCFE* by using the above model.

2.1.2 Model 2

Washing behaviour of pulp fibers in one dimension transport phenomenon of porous media involves axial dispersion and molecular diffusion. The transport equation describing material balance across the bed in one dimension is defined as:

$$D_L\frac{\partial^2 c}{\partial z^2} = u\frac{\partial c}{\partial z} + \frac{\partial c}{\partial t} + \frac{(1-\varepsilon)}{\varepsilon}\frac{\partial n}{\partial t} \qquad (5)$$

Here, the first term represents diffusion dispersion; the other terms represent convective flow, concentration gradient of fluid and concentration gradient of particles respectively.

Mathematically, u and D_L are functions of z, while c and n are functions of both z and t .It is assumed that the deposition rate of solute is of second order in forward direction and detachment rate is of first order in reverse direction. At equilibrium, the monovalent adsorption equation simplifies to nonlinear Langmuir adsorption isotherm as follows:

$$n = \frac{A_0 c}{1 + B_0 c} \tag{6}$$

Where A_0 and B_0 are Langmuir constants.

At the inlet to the packed bed, Robin condition is assumed, *i.e.*, there be no loss of solute from the bed through the plane at which the displacing fluid is introduced, therefore,

$$u\left(c - C_S\right) = D_L \frac{\partial c}{\partial z} \qquad \text{at } z = 0 \ \& \ t > 0 \tag{7}$$

At the exit of the bed, to avoid the unacceptable conclusion that the solute concentration passes through a maximum (or minimum) in the interior of the medium, it is necessary to impose the Neumann boundary condition, *i.e.*,

$$\frac{\partial c}{\partial z} = 0 \qquad \text{at } z = L \ \& \ t > 0 \tag{8}$$

The initial solute concentration is given by:

$$c\left(z, 0\right) = C_0 \tag{9}$$

The solution technique *CHCM* for this model is described by Ganaie *et al* (2013) and Mittal *et al* (2013) with the condition that the concentration of the solute adsorbed on fibers is linked with the concentration of the solute in the flowing liquor via linear and Langmuir adsorption isotherms. The linear isotherm assumes that point-wise equilibrium is attained instantaneously inside the particle, *i.e.*

$$n = kc \tag{10}$$

The Langmuir isotherm assumes that the deposition (adsorption) rate is second order in forward direction and the detachment (desorption) rate is first order in backward direction, *i.e.*,

$$\frac{k_1 c}{C_F}\left(N_i - n\right) - k_2 n = \frac{\partial n}{\partial t} \tag{11}$$

At equilibrium, it simplifies to

$$n = \frac{A_0 c}{1 + B_0 c} \tag{12}$$

where $A_0 = \frac{kN_i}{C_F}$ and $B_0 = \frac{k}{C_F}$

Initially, bulk fluid concentration is taken equal to inlet solute concentration, *i.e.*,

$$c(z,0) = C_i \tag{13}$$

To keep the mathematical complexity as small as possible, the boundary conditions are defined at two points only. One at the top of the bed ($z = 0$) and the other at the bottom of the bed ($z = L$). Between 0 and L, no condition is imposed.

At the inlet of the bed ($z = 0$), the concentration gradient with Danckwert's boundary condition is taken as

$$u(c - C_S) = D_L \frac{\partial c}{\partial z} \tag{14}$$

At the exit of the bed, to avoid the unacceptable conclusion that the solute concentration passes through a maximum (or minimum) in the interior of the medium the concentration gradient is taken as zero i.e.

$$\frac{\partial c}{\partial z} = 0 \qquad \text{at } z = L \ \& \ t > 0 \tag{15}$$

The model based on axial dispersion and particle diffusion describing the washing zone is solved with algorithm based Mathematica & *MATLAB* technique by Potůček (1997 & 2005); Kumar *et al* (2010 & 2013) and Ganaie *et al (*2013) with adsorption isotherm n=kc and the boundary conditions at the inlet and outlet of the bed are (13) and (15). Kukreja & Ray (2009) used (14), (15) and (16) and solved the model for cake washing zone by using Laplace transform.

And the initial conditions is given by

$$c(z,0) = n(z,0) = c_i \text{ for } 0 < z < L/u \tag{16}$$

Brenner (1962) also used the boundary condition (14) and (15). Sherman (1964) used the simple isotherm equation (10). Perron & Lebeau (1977) give the boundary condition at the inlet of the bed $c = c_s$ at z=0 and t>0 and used the isotherm equation:

$$k(c - n) = \frac{\partial n}{\partial t} \tag{17}$$

Kukreja *et al* (1998) used initial and boundary conditions (9), (13) and (18) and adsoption isotherm (17) and solved the above model by using Laplace Transform.

Lapidus & Amundsen (1952) and Kukreja & Ray (2009) used adsorption isotherm which assumes that the deposition rate is constant in forward direction and detachment rate is constant in backward directions i.e. the Finite rate isotherm:

$$k_1 c - k_2 n = \frac{\partial n}{\partial t} \tag{18}$$

Arora *et al* (2008) and Kukreja & Ray (2009) used the conditions (13), (14), (15) and (16) Grähs (1974) Langmuir isotherm. Arora *et al* (2006b) used nonlinear Langmuir adsorption isotherm as follows:

$$n = \frac{ABc}{1+Bc}$$

where A and B are Langmuir constants.

2.1.3 Non-linear Model 3

The displacement washing model based on the axial dispersion and particle diffusion are described earlier by many researchers. The flow of external fluid through a packed bed of fibres is described by one dimensional dispersion plug flow model. The mathematical equation of the model is given:

$$D_L \frac{\partial^2 c}{\partial x^2} = U \frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + C_F \mu \frac{\partial n}{\partial t} \tag{19}$$

with same boundary conditions as discussed above. The concentrations $c(x,t)$ and $n(x,t)$ are related via Langmuir adsorption isotherm as follows:

$$n = \frac{A_0 c}{1+B_0 c} \tag{20}$$

Ma & Guiochon (1991) solved this model by Finite difference method.

The model (19) which is nonlinear in nature is also solved using *MATLAB* 'pdepe' solver. Arora *et al* (2006a) solved this by using Langmuir adsorption isotherm (20) and boundary condition (7) and (8). The author used the initial condition: $c = C_0$, $n = N_0$ at $t = 0$ and $0<z<L$. Ganaie *et al* (2013) have also solved the model with boundary condition and initial condition same but adsorption isotherm (18) with *MATLAB* 'pdepe' solver.

It can be concluded that the *OCFE* with cubic Hermite basis can be applied to linear and nonlinear partial differential equations with equal ease for wide range of parameter *Pe*. The study reveals that the order of convergence using the Gauss Legendre roots is almost double than that of using Chebyshev roots as collocation points. The technique is more consistent than 'pdepe' solver.

2.1.4 Two dimensional Models

The flow of fluid through the pulp bed is described by the bulk fluid concentration denoted by c (z,t). The intrapore concentration is represented by q (r,z,t) and the concentration of solute on the particle surface is n (r,z,t). The particles are cylindrical in nature with pore radius R and porosity of the particle is β. The effective diffusivity and axial dispersion are independent of the cake thickness L and solute concentrations. The relation between bulk fluid and intra-pore diffusion at the particle surface is governed by the fluid film mass transfer coefficient k_f. In the particle diffusion phase the intra-fiber diffusion coefficient

(D_F) is considered only. It is due to the fact that the true surface and solid phase diffusion effects are negligible and are neglected. Hence the transport within a fiber is best described by the diffusion in the solution phase only. The unsteady state partial differential equations for the particle diffusion and bulk fluid are given below:

Mathematical equations for the particle diffusion:

$$D_F\left(\frac{\partial^2 q}{\partial r^2}+\frac{1}{r}\frac{\partial q}{\partial r}\right)-\frac{\partial q}{\partial t}-C_F\frac{(1-\beta)}{\beta}\frac{\partial n}{\partial t}=0 \qquad (21)$$

Boundary conditions: $\frac{\partial q}{\partial r}=0$, at r = 0 (22)

$$\frac{k_f\beta}{K}\left(q\big|_{r=R}-c\right)=-D_F\left(\frac{\partial q}{\partial r}\right), \qquad \text{at r = R} \qquad (23)$$

Adsorption Isotherm: The equation that relates the intra-fiber and inter-fiber solute concentrations is given by Langmuir kinetics. Assuming that the deposition rate is second order in forward direction and detachment rate is first order in reverse direction, following equation is obtained.

$$\frac{\partial n}{\partial t}=k_1\frac{q}{C_F}(N_i-n)-k_2 n \qquad (24)$$

where k_1 and k_2 are deposition and detachment rate constants. At equilibrium this monovalent adsorption equation simplifies to Langmuir adsorption isotherm.

Mathematical equations for the bulk fluid

$$u\varepsilon\frac{\partial c}{\partial z}+\varepsilon\frac{\partial c}{\partial t}+\frac{2(1-\varepsilon)}{R}D_F\left(\frac{\partial q}{\partial r}\right)_{r=R}=D_L\varepsilon\frac{\partial^2 c}{\partial z^2} \qquad (25)$$

Boundary conditions: $uc-D_L\frac{\partial c}{\partial z}=0$, at z = 0 (26)

$$\frac{\partial c}{\partial z}=0, \qquad \text{at z = L} \qquad (27)$$

Initial condition: C = q = C_i and n = N_i at t = 0 (28)

Some authors such as, Arora *et al* (2006a) has used *OCFE* to find the solution of above models. Further, Arora *et al* (2008) and Arora& Potůček (2009) derived the effect of Peclet number and Biot number on exit solute concentration, displacement ratio and efficiency from above models.

Also, Arora & Potůček (2012) used the Mathematical equations for the bulk fluid (25) with same boundary and Initial condition and find the effect of Porosity on exit solute concentration and displacement ratio.

These authors derived excellent results with quadratic convergence using the technique of *OCFE* with cubic Hermite as basis function. Moreover, less computational efforts are required as problems were discretized as a banded matrix with band width two. The method is applicable to linear as well as nonlinear problems with equal ease.

2.2 Recent developments related to the topic

Dyksen & Lynch (2000) used Hermite cubic collocation approximations to find solutions of boundary value problems with either Dirichlet or Neumann boundary conditions.

Arora *et al* (2005) provides the accuracy and stability of *OCFE* used for solving 2-point boundary value problems.

Arora *et al* (2006a) solved one dimensional axial dispersion model for Langmuir adsorption isotherm using the method of *OCFE* and finds the effect of exit solute concentration.

Kukreja & Ray (2009) presented the effect of different parameters in cake formation, washing zone and de-watering zone of microscopic mathematical models

Kumar *et al* (2010) obtained numerical solution of the displacement washing model for the multi-stage counter current manner and used non-linear Langmuir adsorption isotherm. He obtained numerical solutions for four stages and find that boundary conditions do not influence significantly on the washing results.

Arora & Poutcek (2012) applied *OCFE* technique for mathematical model of a displacement washing of craft pulp fiber bed. The authors find the effect of porosity along with Peclet number and Biot number on exit solute concentration.

Ganaie *et al* (2013) evaluated the asymptotic convergence of time-dependent problems such as parabolic partial differential equation using cubic Hermite collocation method. Collocation points are the zeros of Chebyshev polynomials .The solution profiles are converging to zero and the method is asymptotically stable and the cubic Hermite collocation approximations are consistent.

Mittal *et al* (2013) solved the linear and non-linear diffusion-dispersion models by using *OCFE* with cubic Hermite as basis function. The technique is computationally efficient, stable and yield accurate solution.

Kumar *et al* (2013) solved the pulp washing model involving diffusion-dispersion by Separation of variables using *Mathematica* and proved that the present case is giving better results than the previous investigators.

Ganaie *et al* (2013) solved diffusion-dispersion model numerically, using the cubic Hermite collocation method with Gauss Legendre quadrature points of order two, as collocation

points. Linear and nonlinear cases are compared based on experimental data, from a paper mill, reported by previous investigators. It is concluded that the nonlinear isotherm follows the actual desorption process more closely than the linear isotherm.

Arora & Kaur (2014) expressed that in linear case when the collocation points increased from 9 to 11 the relative error is reduced for Pe $\leq$ 20 and when Pe increases, the results do not converge even for large number of collocation points. In case of *OCFE*, the relative error with respect to time and exit solute concentration is less than 1% for just 25 elements when Pe varying from 40 to 100 and in case of *OCM* the relative error is greater than 1% as τ increases from 1.5 even for 19 collocation points. For non-linear advection-diffusion equation, As Pe and Bi increases, wide oscillations are observed at initial stage giving error of more than 4% and for Pe =20.81 and Bi=10 the solution profiles even diverge to negative values as time increases in case of *OCM*. But with *OCFE* using $\|C\|_2$ with 10 elements solution profiles are converging to steady state condition without any oscillation for different values of Pe and Bi.

Ganaie and Kukreja (2014) solved 1D Burgers' equation numerically using Hopf-Cole transformation, which transforms the original nonlinear Burgers' equation into a linear heat equation. The equation is then solved by cubic Hermite spline collocation method by taking Gauss-Legendre quadrature points of order 2 as the collocation points. They also compared the results with exact and numerical results.

Gupta *et al* (2015) solved conveniently nonlinear model representing particle diffusion and molecular diffusion by using cubic spline collocation method and obtained the effect of different parameters on exit solute concentration. Simulation from the model gives that the washing operation is highly sensitive to parameters.

Mittal and Kukreja (2015) solved Mathematical models comprising of non-linear system of partial differential equations related to diffusion dispersion are with the technique of OCFE using cubic Hermite as basis instead of Lagrangian basis. Also author proved that for different values of Peclet numbers (Pe) the rate of convergence is found to be of order 2.

Arora & Kaur (2016) solved the non-linear Burgers' equation directly without transforming it into the linear form using Hopf–Cole transformation with the quintic Hermite collocation method. They used quintic Hermite interpolating polynomials which are of order 5 to approximate the trial function. It is observed that numerical values agree well with the exact ones for *QHCM* as compared to *OCFE*, pdepe solver and *OCM*. These results are shown with the help of plane and surface plots for different values of ε and τ which authenticate the applicability of *QHCM* in solving non-linear stiff system of partial differential equations.

Stability of the *QHCM* has been checked using Euclidian and Supremum norms i.e. with $\|U\|_2$ and $\|U\|_\infty$.

3. Research Gap

A number of mathematical models are available in the literature to describe the complex behaviour of diffusion, dispersion, adsorption, desorption occurring during the solute removal process. Most of the investigators have given various washing models which described linkage between concentrations of solute adsorbed on the fibre surface and the solute present in the liquor. Earlier, *OCM*, *OCFE* and *CHCM* were used in solving these models. As a modification in the technique of *OCFE*, quintic Hermite is used as basis function in the present study. As quintic Hermite are C^2 continuous, so the continuity conditions of trial function and its derivatives at the grid points are satisfied. It is worth mentioning here that this technique reduces mathematical complexity and gives better results. It is evident from the above literature that there is not much work done in the area of quintic Hermite collocation method to solve the boundary value problems as diffusion–diffusion model. Hence to meet the gap, this study is proposed.

4. Problem formulation

Various types of modelling techniques such as process, physical and statistical are generally used for mapping of realistic situations. One of the real-life problems is pulp washing process, in which the mathematical models based on the parameters like axial dispersion and particle diffusion are used. To optimize this, the need of paper & pulp industry is to achieve its target production and also to have a reduced amount of pollution that can be best matched with research on mathematical models. The basic mass transfer relations such as diffusion and material balance equations are used in establishing the models in terms of transport equation. These equations along with adsorption-desorption isotherms, necessary boundary and initial conditions describe the equilibrium between the concentration of the solute in the liquor and concentration of the solute on the fibers. It has been tried to suggest an improvement in the solution of the problem Linear Model 1, Non Linear Model 3 and Two-Dimensional Model for bulk fluid through the proposed method discussed above.

5. Research objectives

Aim of this study is to accurately simulate a packed bed of fibers using mathematical model. Present study has following specific objectives:

a) To build a theoretical framework of two point *BVPs* encountered in industrial practice.
b) To solve the model numerically using orthogonal collocation on finite elements.
c) To make use of quintic Hermite polynomials as basis for discretization of trial function.
d) To use linear and nonlinear adsorption isotherms.
e) To compare the results of quintic Hermite basis *OCFE* with Lagrange's basis *OCFE*, orthogonal collocation method and analytic solution.
f) Collection of the data from literature and laboratory.
g) Simulation of the industrial process using literature and laboratory data.
h) Interpretation of results in terms of conventional parameters used in industry.

6. Contribution and need of the proposed research

Pulp washing is a process to recover clean pulp and remove maximal amount of solutes with amount of water as little as possible. The mechanism of solute removal is associated with diffusion like dispersion models. The proposed method solves these models using less computational work and time.

7. Methodology

In the present study, the method of orthogonal collocation on finite elements using quintic Hermite basis is applied to different linear and nonlinear models in one dimensional space.
In this method, the domain $0 \le \zeta \le 1$ is divided into finite number of sub regions called elements by inserting $\zeta_1, \zeta_2, ..., \zeta_{N+1}$ points such that $0=\zeta_1 < \zeta_2 < \ldots\ldots < \zeta_{N+1} = 1$ with $h_k = \zeta_{k+1} - \zeta_k$. Introducing a new variable $u = (\zeta - \zeta_k)/h_k$ such that u varies from 0 to1 when ζ varies from ζ_k to ζ_{k+1} .Then apply orthogonal collocation method with quantic Hermite as basis function within each element.

Approximate solution $c(u,t)$ at the r^{th} collocation point in the q^{th} element is given by:

$$c_{qr}(u,t) = \sum_{p=1}^{6} \alpha_{p+2(q-1)}^{qr}(t) H_p^q(u);\ q = 1,2,...,k;\ r = 2,3,4,5. \tag{29}$$

$$\frac{\partial c_{qr}}{\partial u} = \frac{1}{h_q} \sum_{l=1}^{6} \alpha_{p+2(q-1)}^{qr} \frac{dH_p^q}{du} \tag{30}$$

$$\frac{\partial^2 c_{qr}}{\partial u^2} = \frac{1}{h_q^2} \sum_{p=1}^{6} a_{p+2(q-1)}^{qr} \frac{d^2 H_p^q}{du^2} \tag{31}$$

$$\frac{\partial c_{qr}}{\partial t} = \sum_{l=1}^{6} \frac{da_{p+2(q-1)}^{qr}}{dt} H_p^q \tag{32}$$

Where the standard quintic Hermite basis functions H_p^q 's are given by:

$$H_{3p-2}^q(\xi) = \begin{cases} \left(\frac{\xi-\xi_{q-1}}{h_{q-1}}\right)^3 \left(6\left(\frac{\xi-\xi_{q-1}}{h_{q-1}}\right)^2 - 15\left(\frac{\xi-\xi_{q-1}}{h_{q-1}}\right) + 10\right); & \xi \in [\xi_{q-1}, \xi_q] \\ \left(1-\frac{\xi-\xi_q}{h_q}\right)^3 \left(1+3\left(\frac{\xi-\xi_q}{h_q}\right) + 6\left(\frac{\xi-\xi_q}{h_q}\right)^2\right); & \xi \in [\xi_q, \xi_{q+1}] \\ 0; & \textit{otherwise} \end{cases} \tag{33}$$

$$H_{3p-1}^q(\xi) = \begin{cases} -h_{q-1}\left(\frac{\xi-\xi_{q-1}}{h_{q-1}}\right)^3 \left(1-\frac{\xi-\xi_{q-1}}{h_{q-1}}\right)\left(4-3\frac{\xi-\xi_{q-1}}{h_{q-1}}\right); & \xi \in [\xi_{q-1}, \xi_q] \\ h_q\left(1-\frac{\xi-\xi_q}{h_q}\right)^3 \left(\frac{\xi-\xi_q}{h_q}\right)\left(1+3\frac{\xi-\xi_q}{h_q}\right); & \xi \in [\xi_q, \xi_{q+1}] \\ 0; & \textit{otherwise} \end{cases} \tag{34}$$

$$H_{3p}^q(\xi) = \begin{cases} \frac{1}{2}h_{q-1}\left(\frac{\xi-\xi_{q-1}}{h_{q-1}}\right)^3 \left(1-\frac{\xi-\xi_{q-1}}{h_{q-1}}\right)^2; & \xi \in [\xi_{q-1}, \xi_q] \\ \frac{1}{2}h_q\left(1-\frac{\xi-\xi_q}{h_q}\right)^3 \left(\frac{\xi-\xi_q}{h_q}\right)^2; & \xi \in [\xi_q, \xi_{q+1}] \\ 0; & \textit{otherwise} \end{cases} \tag{35}$$

The trial function is comprised of value of the function and first derivative at each end in such a manner that five of these quantities are zero and sixth is one. In particular, for k^{th} element $[\zeta_k, \zeta_{k+1}]$ quintic Hermite basis functions are given as follows:

$$\left.\begin{aligned} H_1^k(\xi) &= \left(1+3\xi+6\xi^2\right)\left(1-\xi\right)^3 \\ H_2^k(\xi) &= \xi\left(1-\xi\right)^3\left(1+3\xi\right) \\ H_3^k(\xi) &= \frac{1}{2}\xi^2\left(1-\xi\right)^3 \\ H_4^k(\xi) &= \xi^3\left(6\xi^2-15\xi+10\right) \\ H_5^k(\xi) &= \xi^3\left(1-\xi\right)\left(3\xi-4\right) \\ H_6^k(\xi) &= \frac{1}{2}\xi^3\left(1-\xi\right)^2 \end{aligned}\right\} \tag{36}$$

The zeros of Gauss-Legendre polynomials are taken as collocation points because these polynomials have the tendency to reduce error to minimum (Fan, *et al* 1971; Finlayson (1980)) and yield satisfactory results.

Generally two types of basis are used for approximating the solution at the collocation points, Lagrange basis and Hermite basis. In the present study, the technique of *OCFE* with quantic Hermite basis will be used for the solution as the technique of orthogonal collocation on finite elements using quantic Hermite basis which is C^2 continuous is quite useful than orthogonal collocation method and orthogonal collocation on finite elements. This technique has the advantage that it reduces the number of equations because of C^1 continuity of Hermite polynomials. The model will be solved using *MATLAB* 'pdepe' solver.

The data will be collected from a paper Industry and will be analysed in the laboratory. The mathematical model is of significance if it can be implemented in the Industry. The model proposed in the present study will be also correlated with efficiency parameters which are measured form the model using average solute concentration. The effects of different parameters such as peclet numbers, cake thickness, interstitial velocity, bed porosity, and distribution ratio will be checked on exit solute concentration and average solutes concentration. Also the results obtained from the model will be presented in the form of break-through curves i.e. dimensionless concentration vs. dimensionless time graph.

8. Place of work

a) Maharaja Ranjit Singh Punjab Technical University, Bathinda, Punjab
b) Sant Longowal Institute of Engg. & Technology, Longowal, Sangrur, Punjab - Co-supervisor's place of work.

9. Resources required and availability status

Software required – MATLAB; MathType; LaTeX Typesetting.

Available at the place of work.

Bibliography

1. Al-Jabari, M., Van Heiningen, A. R. P., & Van De Ven, T. G. M. (1994). Modelling the flow and the deposition of fillers in packed beds of pulp fibres. *Journal of pulp and paper science*, *20*(9), J249-J253.
2. Arora, S., Dhaliwal, S. S., & Kukreja, V. K. (2005). Solution of two point boundary value problems using orthogonal collocation on finite elements. *Applied mathematics and computation*, *171*(1), 358-370.

3. Arora, S., Dhaliwal, S. S., & Kukreja, V. K. (2006a). Simulation of washing of packed bed of porous particles by orthogonal collocation on finite elements. *Computers & chemical engineering*, *30*(6-7), 1054-1060
4. Arora, S., Dhaliwal, S. S., & Kukreja, V. K. (2006b). Application of orthogonal collocation on finite elements for solving non-linear boundary value problems. *Applied mathematics and computation*, *180*(2), 516-523.
5. Arora, S., Dhaliwal, S. S., & Kukreja, V. K. (2008). Mathematical modelling of the washing zone of an industrial rotary vacuum washer. *Indian Journal of Chemical Technology*, 15, 332-340.
6. Arora, S., & Potůček, F. (2009). Modelling of displacement washing of packed bed of fibers. *Brazilian Journal of Chemical Engineering*, *26*(2), 385-393.
7. Arora, S., Kaur, I. (2014). Numerical Solutions of Two Point Boundary Value Problems Using Collocation Techniques. *International Journal of Scientific & Engineering Research, 5*(1), 718-726.
8. Arora, S., & Kaur, I. (2016). An efficient scheme for numerical solution of Burgers' equation using quintic Hermite interpolating polynomials. *Arabian Journal of Mathematics*, *5*(1), 23-34.
9. Arora, S., & Potůček, F. (2012). Verification of mathematical model for displacement washing of kraft pulp fibres. *Indian Journal of Chemical Technology*, *19*, 140-148.
10. Brenner, H. (1962). The diffusion model of longitudinal mixing in beds of finite length. Numerical values. *Chemical Engineering Science*, *17*(4), 229-243.
11. Carey, G. F., & Finlayson, B. A. (1975). Orthogonal collocation on finite elements. *Chemical Engineering Science*, *30*(5-6), 587-596.
12. Dyksen, W. R., & Lynch, R. E. (2000). A new decoupling technique for the Hermite cubic collocation equations arising from boundary value problems. *Mathematics and Computers in Simulation*, *54*(4-5), 359-372.
13. Fan, L. T., Chen, G. K. C., & Erickson, L. E. (1971). Efficiency and utility of collocation methods in solving the performance equations of flow chemical reactors with axial dispersion. *Chemical Engineering Science*, *26*(3), 378-387.
14. Finlayson, B. A. (1971). Packed bed reactor analysis by orthogonal collocation. *Chemical Engineering Science*, *26*(7), 1081-1091.
15. Finlayson, B. A. (1980). *Nonlinear analysis in chemical engineering*. McGraw-Hill Inc, USA.

16. Ganaie, I. A., Gupta, B., Parumasur, N., Singh, P., & Kukreja, V. K. (2013). Asymptotic convergence of cubic Hermite collocation method for parabolic partial differential equation. *Applied Mathematics and Computation*, *220*, 560-567.
17. Ganaie, I. A., & Kukreja, V. K. (2014). Numerical solution of Burgers' equation by cubic Hermite collocation method. *Applied Mathematics and Computation*, *237*, 571-581.
18. Grähs, L. E. (1974). *Washing of cellulose fibres: analysis of the displacement washing operation*. PhD Thesis, Chalmers University of Technology, Goteborg, Sweden.
19. Gupta, B., & Kukreja, V. K. (2012). Numerical approach for solving diffusion problems using cubic B-spline collocation method. *Applied Mathematics and Computation*, *219*(4), 2087-2099.
20. Gupta, B., Kukreja, V. K., Parumasur, N., & Singh, P. (2015). Numerical Study of a Nonlinear Diffusion Model for Washing of Packed Bed of Cylindrical Fiber Particles. *Arabian Journal for Science and Engineering*, *40*(5), 1279-1287.
21. Kim, D. H. (1989). Linear driving force formulas for diffusion and reaction in porous catalysts. *AIChE journal*, *35*(2), 343-346.
22. Kukreja, V. K., Ray, A. K., & Singh. V. P. (1998). Mathematical models for washing and dewatering zones of a rotary vacuum filter. *Indian Journal of Chemical Technology*, 5, 276-280.
23. Kukreja, V. K., Ray, A. K., Singh, V. P., & Rao, N. J. (1995). A Mathematical model for pulp washing in different zones of a rotary vacuum filter, *Journal of Indian Institute of Chemical Engineers*, *37*, 113-124.
24. Kukreja, V. K., & Ray, A. K. (2009). Mathematical modelling of a rotary vacuum washer used for pulp washing: a case study of a lab scale washer. *Cellulose Chemistry & Technology*, *43*(1), 25.
25. Kumar, D., Kumar, V., & Singh, V. P. (2010). Mathematical modelling of brown stock washing problems and their numerical solution using MATLAB. *Computers & Chemical Engineering*, *34*(1), 9-16.
26. Kumar, J., Ganaie, I. A., & Kukreja, V. K. (2013). Application of Mathematica software to solve pulp washing model. *ISRN Chemical Engineering*, *2013*.
27. Kuo, M. T. (1960). Filter cake washing performance. *AIChE Journal*, *6*(4), 566-568.
28. Liao, H. T., & Shiau, C. Y. (2000). Analytical solution to an axial dispersion model for the fixed-bed adsorber. *AIChE Journal*, *46*(6), 1168-1176.

29. Lapidus, L., & Amundson, N. R. (1952). Mathematics of adsorption in beds. VI. The effect of longitudinal diffusion in ion exchange and chromatographic columns. *The Journal of Physical Chemistry*, *56*(8), 984-988.
30. Liu, F., & Bhatia, S. K. (1999). Computationally efficient solution techniques for adsorption problems involving steep gradients in bidisperse particles. *Computers & Chemical Engineering*, *23*(7), 933-943.
31. Ma, Z., & Guiochon, G. (1991). Application of orthogonal collocation on finite elements in the simulation of non-linear chromatography. *Computers & Chemical Engineering*, *15*(6), 415-426.
32. Mittal, A. K., Ganaie, I. A., Kukreja, V. K., Parumasur, N., & Singh, P. (2013). Solution of diffusion–dispersion models using a computationally efficient technique of orthogonal collocation on finite elements with cubic Hermite as basis. *Computers & Chemical Engineering*, *58*, 203-210.
33. Mittal, A., & Kukreja, V. K. (2015). Convergence of Orthogonal collocation on finite elements with Hermite basis method for two dimensional nonlinear models. *International Journal of Mathematical Sciences and Applications*, *5*(1), 187-192.
34. Neretnieks, I. (1976). Adsorption in finite bath and counter current flow with systems having a nonlinear isotherm. *Chemical Engineering Science*, *31*(2), 107-114.
35. Onah, S. E. (2002). Asymptotic behaviour of the Galerkin and the finite element collocation methods for a parabolic equation. *Applied Mathematics and Computation*, *127*(2-3), 207-213.
36. Pekkanen, M., & Norden, H. V. (1985). Review of pulp washing models. *Paperi ja puu*, *67*(11), 689-696.
37. Pellett, G. L. (1964). *Longitudinal dispersion, intrafiber diffusion, and liquid-phase mass transfer during flow through fiber beds.* PhD Thesis, Georgia Institute of Technology, Georgia.
38. Perron, M., & Lebeau, B. (1977). A mathematical model of pulp washing on rotary drums. *Pulp and paper Canada*, *78*(3), TR1-TR5.
39. Potůček, F. (1997). Washing of pulp fibre bed. *Collection of Czechoslovak Chemical Communications*, *62*(4), 626-644.
40. Potůček, F. (2001). Displacement of washing of pulp II. Analysis of laboratory data. *Papir a Celulóza*, 56(2), 49-53.
41. Potůček, F. (2005). Chemical engineering view of the pulp washing. *Papir a celulóza*, *60*(4), 114-117.

42. Prenter, P. M. (1975). *Splines and variational methods*. John Wiley & Sons, New York.
43. Raghavan, N. S., & Ruthven, D. M. (1983). Numerical simulation of a fixed-bed adsorption column by the method of orthogonal collocation. *AIChE Journal*, *29*(6), 922-925.
44. Rasmuson, A., & Neretnieks, I. (1980). Exact solution of a model for diffusion in particles and longitudinal dispersion in packed beds. *AIChE Journal*, *26*(4), 686-690.
45. Sherman, W. R. (1964). The movement of a soluble material during the washing of a bed of packed solids. *AIChE Journal*, *10*(6), 855-860.
46. Shiraishi, F. (2001). Highly accurate solution of the axial dispersion model expressed in S-system canonical form by Taylor series method. *Chemical Engineering Journal*, *83*(3), 175-183.
47. Soliman, M. A., & Ibrahim, A. A. (1999). Studies on the method of orthogonal collocation III: the use of Jacobi orthogonal polynomials for the solution of boundary value problems. *Journal of King Saud University*, *11*(2), 191-202.
48. Sridhar, P. (1999).Implementation of the one point orthogonal collocation method to an affinity packed bed model. *Indian Chemical Engineering*, *41*(1), 39–46.
49. Sun, W. (2000). Hermite cubic spline collocation methods with upwind features. *ANZIAM journal, 42*, 1379-1397.
50. Szukiewicz, M. K. (2000). New approximate model for diffusion and reaction in a porous catalyst. *AIChE Journal*, *46*(3), 661-665.
51. Trinh, D. T., Poirier, N. A., Crotogino, R. H., & Douglas, W. J. M. (1989). Displacement washing of wood pulp. An experimental study. *Journal of Pulp and Paper Science*, *15*(1), J28-J35.
52. Villadsen, J. V., & Stewart, W. E. (1967). Solution of boundary-value problems by orthogonal collocation. *Chemical Engineering Science*, *22*(11), 1483-1501.